# The Importance of Boundary Conditions in Quantum Mechanics

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**Abstract.** We discuss the role of boundary conditions in determining the physical content of the solutions of the Schrödinger equation. We study the standing-wave, the "in," the "out," and the purely outgoing boundary conditions. As well, we rephrase Feynman's $+i\varepsilon$ prescription as a time-asymmetric, causal boundary condition, and discuss the connection of Feynman's $+i\varepsilon$ prescription with the arrow of time of Quantum Electrodynamics. A parallel of this arrow of time with that of Classical Electrodynamics is made. We conclude that in general, the time evolution of a closed quantum system has indeed an arrow of time built into the propagators.

## 1 Introduction

In physics, dynamical equations often have a differential form and are solved under various boundary conditions. This is also the case in Quantum Mechanics, whose dynamics is encoded by the Schrödinger equation. The purpose of this contribution is to discuss, in a somewhat sketchy way, how boundary conditions imposed upon the Schrödinger equation determine the physical content of its solutions. And vice versa: in order to obtain the solutions of the Schrödinger equation that describe a given physical situation, boundary conditions that fit the physical situation must be imposed upon the Schrödinger equation.

In the non-relativistic domain, the time-independent Schrödinger equation is realized, in the position representation, as a second-order differential equation. If the potential is simple enough, we can exactly solve the differential equation by means of the Sturm-Liouville theory [1–3]. This theory yields an eigenfunction expansion, a unitary operator that diagonalizes the Hamiltonian, and a direct integral decomposition. In its turn, the direct integral decomposition yields, along with some physical requirements, a Rigged Hilbert Space (RHS). The eigenfunction expansion, the unitary operator that diagonalizes the Hamiltonian, the direct integral decomposition, and the RHS contain much of the spectral and physical informations of the Hamiltonian. For convenience, we shall refer to them as the RHS properties (abbreviated RSP) associated to the Hamiltonian [4]. At first sight, it may seem that the Schrödinger equation corresponding to a given Hamiltonian generates just one single RSP. However, this is not necessarily so. There are certain types of boundary conditions that, when imposed upon the Schrödinger equation, yield different RSPs. To be more precise, the standing-wave boundary condition (to be defined below), and the "in" and "out" boundary conditions of the Lippmann-Schwinger equation generate three different RSPs.

The Gamow vectors are the state vectors of resonances [5–10,1]. Like the standing-wave and the Lippmann-Schwinger eigensolutions, they solve the Schrödinger equation. At infinity, however, the Gamow eigenfunctions satisfy the purely outgoing boundary condition. This condition selects the (complex) resonance spectrum of the Schrödinger equation.

The time-dependent Schrödinger equation is time symmetric, the reason for which it is generally believed that Quantum Mechanics is time symmetric [11]. And yet the time evolution of individual atoms or subatomic particles seems to have some directness. For example, imagine that we want to compute the probability for a particle to go from an initial space-time location $(\mathbf{x},t)$ to a final space-time location $(\mathbf{x}',t')$. Our basic notions of causality dictate that this probability be zero when $t'<t$. However, as far as the Schrödinger equation is concerned, this probability is also non-zero when $t'<t$. In order to obtain the causal result, we have to use the retarded propagator $G^+(\mathbf{x},t;\mathbf{x}',t')$ (see for example [12]). This retarded propagator automatically yields a causal probability, because it vanishes when $t'<t$:

$$G^+(\mathbf{x},t;\mathbf{x}',t')=0\,, \quad t'<t\,. \tag{1}$$

Therefore, the time evolution given by $G^+(\mathbf{x},t;\mathbf{x}',t')$ has an arrow of time: a particle travels forward in time, never backward. As is well known, the time evolution given by the (e.g., retarded) propagator is equivalent to the time-dependent Schrödinger equation subject to an (e.g., retarded) causal boundary condition. Hence, the arrow of time built into $G^+(\mathbf{x},t;\mathbf{x}',t')$ stems ultimately from causal boundary conditions.

Quantum Electrodynamics (QED) provides a glaring example of how the propagators carry an arrow of time. In QED, the Feynman propagator is constructed by imposing Feynman's $+\mathrm{i}\varepsilon$ prescription upon the time evolution of particles and antiparticles [13]. Particles travel forward in time, whereas antiparticles "travel backward" in time. Clearly, this prescription builds an arrow of time into the Feynman propagator. But note that this arrow of time is introduced by means of Feynman's $+\mathrm{i}\varepsilon$ prescription, which is a boundary condition. Thus, the arrow of time of the Feynman propagator also stems ultimately from causal boundary conditions.

The organization of this contribution is as follows:

(*i*) In order to obtain the standing-wave eigensolution $\langle r|E\rangle$, the "in" Lippmann-Schwinger eigensolution $\langle r|E^+\rangle$, and the "out" Lippmann-Schwinger eigensolution $\langle r|E^-\rangle$, we shall impose upon the Schrödinger equation the standing-wave, the "in," and the "out" boundary condition, respectively. Each of the eigensolutions $\langle r|E\rangle$, $\langle r|E^+\rangle$, $\langle r|E^-\rangle$ yields an RSP of its own. Hence, we shall conclude that each of the eigensolutions $\langle r|E\rangle$, $\langle r|E^+\rangle$, $\langle r|E^-\rangle$ has a physical content of its own.

(*ii*) It will be apparent that what makes $\langle r|E\rangle$, $\langle r|E^+\rangle$, $\langle r|E^-\rangle$ different from each other is the boundary conditions that they satisfy. More precisely, what makes them different from each other is their asymptotic behavior at infinity.

(*iii*) We will relate the asymptotic behavior at infinity of $\langle r|E\rangle$, $\langle r|E^+\rangle$, $\langle r|E^-\rangle$ with their analytical dependence on the energy, and see why applying the Sturm-Liouville theory to these eigenfunctions yields three different RSPs.

(*iv*) When two eigenfunctions have just a different normalization, they generate the same RSP. A criterion to check whether or not two eigensolutions lead to different RSPs (i.e., whether or not two eigensolutions differ from a normalization factor) is provided. We shall apply the criterion to $\langle r|E\rangle$, $\langle r|E^+\rangle$, $\langle r|E^-\rangle$ and see (as expected) that they are not a normalization of each other.

(*v*) We shall compare the boundary conditions satisfied by the Gamow vectors with those satisfied by $\langle r|E\rangle$, $\langle r|E^+\rangle$, and $\langle r|E^-\rangle$. More precisely, we shall compare the purely outgoing boundary condition with the standing-wave, "in," and "out" boundary conditions, and see why the purely outgoing boundary condition determines the physical content of the Gamow vectors.

(*vi*) We shall discuss the time asymmetry of QED. We shall refer to this time asymmetry as the QED arrow of time. We shall see that the QED arrow of time is built into Feynman's propagator. A parallel of the QED arrow of time with that of Classical Electrodynamics will be made. We shall conclude that, in general, there exists an arrow of time at the microscopic level, and that this arrow of time arises from the imposition of a time-asymmetric, causal boundary condition upon the (time-symmetric) Schrödinger equation. Because solving the Schrödinger equation subject to a time-asymmetric boundary condition necessarily involves the construction of a propagator, we shall conclude that the quantum-mechanical arrow of time is built into the propagators.

## 2 Boundary Conditions upon the Time-Independent Schrödinger Equation

We proceed now to see how boundary conditions affect the behavior of the solutions of the time-independent Schrödinger equation. Rather than working in a general fashion, we shall use the spherical shell potential as an illustrative example. Generalizations to more complicated potentials are straightforward.

Consider the spherical shell potential of height $V_0$,

$$V(\boldsymbol{x}) = V(r) = \begin{cases} 0 & 0<r<a \\ V_0 & a<r<b \\ 0 & b<r<\infty\,. \end{cases} \tag{2}$$

If we restrict ourselves to the zero angular momentum case, then the spherical shell Hamiltonian acts, in the radial position representation, as the following formal differential operator:

$$h \equiv -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V(r)\,. \tag{3}$$

The time-independent Schrödinger equation (for zero angular momentum) reads

$$\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V(r)\right)\sigma(r;E) = E\sigma(r;E)\,. \tag{4}$$

Our objective in this section is to solve (4) subject to various boundary conditions, and to analyze the physical content of both the solutions and the boundary conditions. We shall study three cases: the standing-wave, the Lippmann-Schwinger, and the Gamow eigensolutions.

### 2.1 Standing-Wave Eigenfunctions

We first study the standing-wave eigenfunctions. To obtain them, we solve (4) under the following boundary conditions:

$$\sigma(0;E) = 0\,, \tag{5a}$$
$$\sigma(r;E) \text{ is continuous at } r=a \text{ and at } r=b\,, \tag{5b}$$
$$\frac{\mathrm{d}}{\mathrm{d}r}\sigma(r;E) \text{ is continuous at } r=a \text{ and at } r=b\,. \tag{5c}$$

The eigensolution of (4) that satisfies (5a)–(5c) is given by the regular solution:

$$\chi(r;E) \equiv \chi(r;k) = \begin{cases} \sin(kr) & 0<r<a \\ \mathcal{J}_1(k)\mathrm{e}^{\mathrm{i}Qr} + \mathcal{J}_2(k)\mathrm{e}^{-\mathrm{i}Qr} & a<r<b \\ \mathcal{J}_3(k)\mathrm{e}^{\mathrm{i}kr} + \mathcal{J}_4(k)\mathrm{e}^{-\mathrm{i}kr} & b<r<\infty\,, \end{cases} \tag{6}$$

where

$$k = \sqrt{\frac{2m}{\hbar^2}E}\,, \quad Q = \sqrt{\frac{2m}{\hbar^2}(E-V_0)}\,. \tag{7}$$

The coefficients $\mathcal{J}_1(k)$–$\mathcal{J}_4(k)$ in (6) are such that $\chi(r;E)$ satisfies (5b) and (5c). The expressions of $\mathcal{J}_1(k)$–$\mathcal{J}_4(k)$ can be easily calculated (they can also be found, for example, in [1]).

The regular solution $\chi(r;E)$ is not $\delta$-normalized. In order to $\delta$-normalize it, we need the spectral measure

$$\varrho(E) \equiv \varrho(k) = \frac{1}{4\pi}\,\frac{2m/\hbar^2}{k}\,\frac{1}{|\mathcal{J}_4(k)|^2}\,. \tag{8}$$

Multiplying $\chi(r;E)$ by the square root of this spectral measure yields the $\delta$-normalized eigensolution of (4) that satisfies the boundary conditions (5a)–(5c):

$$\langle r|E\rangle \equiv \sqrt{\varrho(k)}\,\chi(r;k)\,. \tag{9}$$

The $\delta$-normalization of $\langle r|E\rangle$ is to be understood in the following sense:

$$\int_0^\infty \mathrm{d}r \, \langle E|r\rangle\langle r|E'\rangle = \delta(E-E') \, , \quad E, E' \in [0,\infty) \, , \tag{10}$$

where $\langle E|r\rangle$ is the complex conjugate of $\langle r|E\rangle$. Note that although $\langle r|E\rangle$ is also defined for complex energies, we have restricted $E$ to $[0,\infty)$, because the (Hilbert space) spectrum of the Hamiltonian (3) is the positive real line.

At infinity, the eigensolution (9) is a linear combination of

$$\sqrt{\varrho(k)}\, \mathcal{J}_4(k)\, \mathrm{e}^{-\mathrm{i}kr} \, , \tag{11}$$

which is an incoming spherical wave of amplitude $\sqrt{\varrho(k)}\, \mathcal{J}_4(k)$, and

$$\sqrt{\varrho(k)}\, \mathcal{J}_3(k)\, \mathrm{e}^{\mathrm{i}kr} \, , \tag{12}$$

which is an outgoing spherical wave of amplitude $\sqrt{\varrho(k)}\, \mathcal{J}_3(k)$. It is easy to see that when $E$ is real, (11) is the complex conjugate of (12). Thus, far away from the potential region, $\langle r|E\rangle$ is the linear combination of an incoming spherical wave and its complex conjugate. This behavior is very much like that of a sinusoidal function – hence the name standing-wave solution for the eigenfunction $\langle r|E\rangle$.

As shown in [1], the eigenfunctions (9) generate, by means of the Sturm-Liouville theory,[1] an RSP; that is, the $\langle r|E\rangle$ generate an eigenfunction expansion, a unitary operator $U$ that diagonalizes the Hamiltonian, a direct integral decomposition, and an RHS

$$\boldsymbol{\Phi} \subset \mathcal{H} \subset \boldsymbol{\Phi}^\times \, . \tag{13}$$

(The explicit form of the RSP generated by the eigenfunctions (9) can be found in [1].) Now, the boundary conditions (5a)–(5c) completely determine the radial dependence of the eigensolution of the Schrödinger equation (4). Essentially, the regular solution $\chi(r;E)$ is unique up to multiplication by a function of the energy. Since in Quantum Mechanics the boundary conditions (5a)–(5c) are customarily imposed upon the Schrödinger equation, one may be tempted to conclude that we have found all the possible RSPs of the spherical shell potential. As we shall see, this is not the case: when we multiply $\chi(r;E)$ by the Jost functions, we obtain the "in" and "out" eigensolutions, which generate two new RSPs for the spherical shell potential. The "in" and "out" eigensolutions (and therefore their associated RSPs) are determined by the boundary conditions built into the Lippmann-Schwinger equation.

### 2.2 Lippmann-Schwinger Eigenfunctions

The Lippmann-Schwinger equation is usually written as

$$|E^\pm\rangle = |E\rangle + \frac{1}{E - H_0 \pm \mathrm{i}\varepsilon} V |E^\pm\rangle \, , \tag{14}$$

[1] Our basic reference on the Sturm-Liouville theory is [14]. Illustrative applications of the Sturm-Liouville theory can be found, for example, in [1–3,15–17].

where $H_0$ is the free Hamiltonian. In the radial position representation, (14) reads

$$\langle r|E^{\pm}\rangle = \langle r|E\rangle + \langle r|\frac{1}{E-H_0 \pm \mathrm{i}\varepsilon} V|E^{\pm}\rangle \, . \tag{15}$$

The solutions $\langle r|E^{\pm}\rangle$ of this equation will be called the "in" (+) and "out" (−) Lippmann-Schwinger eigenfunctions. As is well known, the integral equation (15) is equivalent to the Schrödinger equation

$$\left( -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V(r) \right) \langle r|E^{\pm}\rangle = E\langle r|E^{\pm}\rangle \tag{16}$$

subject to the following boundary conditions:

$$\langle 0|E^{\pm}\rangle = 0 \, , \tag{17a}$$

$$\langle r|E^{\pm}\rangle \text{ is continuous at } r=a \text{ and at } r=b \, , \tag{17b}$$

$$\frac{\mathrm{d}}{\mathrm{d}r}\langle r|E^{\pm}\rangle \text{ is continuous at } r=a \text{ and at } r=b \, , \tag{17c}$$

$$\langle r|E^{+}\rangle \sim \mathrm{e}^{-\mathrm{i}kr} - S(k)\mathrm{e}^{\mathrm{i}kr} \quad \text{as } r\to\infty \, , \tag{17d}$$

$$\langle r|E^{-}\rangle \sim \mathrm{e}^{\mathrm{i}kr} - S^*(k)\mathrm{e}^{-\mathrm{i}kr} \quad \text{as } r\to\infty \, , \tag{17e}$$

where $S(k)$ is the $S$ matrix, which is given by the quotient of the Jost functions:

$$S(E) \equiv S(k) = \frac{\mathcal{J}_-(k)}{\mathcal{J}_+(k)} \, . \tag{18}$$

The Jost functions can be written in terms of the coefficients of (6) as

$$\mathcal{J}_+(k) = -2i\mathcal{J}_4(k) \, ; \quad \mathcal{J}_-(k) = 2i\mathcal{J}_3(k) \, . \tag{19}$$

The $\delta$-normalized [in the sense of (10)] Lippmann-Schwinger eigenfunctions can be easily obtained from (16)–(19):

$$\langle r|E^{\pm}\rangle = \sqrt{\varrho^{\pm}(k)}\,\frac{\chi(r;k)}{\mathcal{J}_{\pm}(k)} \, , \tag{20}$$

where $\varrho^{\pm}(k)$ are spectral measures,

$$\varrho^{+}(k) = \varrho^{-}(k) = \frac{1}{\pi}\,\frac{2m/\hbar^2}{k} \, . \tag{21}$$

As in the standing-wave case, we are restricting $E$ to $[0,\infty)$. From (18), (20) and (21) it follows that the Lippmann-Schwinger eigenfunctions are proportional to each other:

$$\langle r|E^{+}\rangle = S(E)\,\langle r|E^{-}\rangle \, . \tag{22}$$

Applying the Sturm-Liouville theory to $\langle r|E^{\pm}\rangle$ yields two other RSPs [1], i.e., two eigenfunction expansions, two unitary operators $U_{\pm}$ that diagonalize the Hamiltonian, two direct integral decompositions, and two RHSs[2]

$$\mathbf{\Phi}_{\pm} \subset \mathcal{H} \subset \mathbf{\Phi}_{\pm}^{\times} \, . \tag{23}$$

[2] The RHSs (23) are sketched in [1]. Their complete characterization is a matter of current investigation.

Therefore, even though $\langle r|E\rangle$, $\langle r|E^+\rangle$, $\langle r|E^-\rangle$ all fulfill one and the same Schrödinger equation and have one and the same radial dependence, they generate three different RSPs. Moreover, $\langle r|E^+\rangle$ and $\langle r|E^-\rangle$ differ from each other by just a phase factor [see (22)], because $|S(E)| = 1$ when $E \in [0, \infty)$. How is then possible that they lead to different RSPs? The answer to this question is the following: $\langle r|E\rangle$, $\langle r|E^+\rangle$, $\langle r|E^-\rangle$ lead to different RSPs because they satisfy different, physically non-equivalent boundary conditions.

In order to better understand why $\langle r|E\rangle$, $\langle r|E^+\rangle$, $\langle r|E^-\rangle$ yield three different RSPs, we compare the Lippmann-Schwinger boundary conditions (17a)–(17e) to the standing-wave boundary conditions (5a)–(5c). We can see first that the boundary conditions (17a)–(17c) are the same as (5a)–(5c). We can also see that in the Lippmann-Schwinger case, we have imposed an additional boundary condition that selects the asymptotic behavior of the eigenfunctions at infinity. For the "in" Lippmann-Schwinger eigenfunction, we have chosen (17d), which means that far away from the potential region $\langle r|E^+\rangle$ is a linear combination of an incoming spherical wave and an outgoing spherical wave multiplied by the $S$ matrix (which is a phase factor). For the "out" Lippmann-Schwinger eigenfunction, we have chosen (17e), which means that far away from the potential region $\langle r|E^-\rangle$ is a linear combination of an outgoing spherical wave and an incoming spherical wave multiplied by the complex conjugate of the $S$ matrix (which is also a phase factor). In the standing-wave case, we did not explicitly impose any boundary condition at infinity, which is tantamount to imposing the standing-wave asymptotic behavior. Thus $\langle r|E\rangle$, $\langle r|E^+\rangle$, $\langle r|E^-\rangle$ differ from each other just by their asymptotic behavior at infinity. These different asymptotic behaviors lead, by means of the Jost functions, to different analytical properties of the eigensolutions as functions of the energy when $E$ is allowed to be complex. Because the Sturm-Liouville theory [14] always deals with complex energies, eigenfunctions with different analytical properties yield different RSPs. Therefore, what ultimately makes $\langle r|E\rangle$, $\langle r|E^+\rangle$, $\langle r|E^-\rangle$ different is their different analytical behavior when $E$ is allowed to be complex.

An important conclusion can be drawn from the previous paragraph: boundary conditions that in the position representation select the asymptotic behavior read, in the energy representation, as boundary conditions that select the analytical behavior, and vice versa. This is particularly apparent in the Lippmann-Schwinger equation, where the asymptotic boundary conditions (17d) and (17e) are built into the $\pm i\varepsilon$ of (15), and vice versa. We then say that the analytical boundary conditions of the Lippmann-Schwinger equation select what is "in" ($+i\varepsilon$) and what is "out" ($-i\varepsilon$) or, equivalently, that the asymptotic behaviors select what is "in" (17d) and what is "out" (17e).

The eigenfunctions $\langle r|E\rangle$, $\langle r|E^+\rangle$, $\langle r|E^-\rangle$ all are proportional to the regular solution $\chi(r;E)$:

$$\langle r|E\rangle = \sqrt{\varrho(k)}\, \chi(r;k)\,, \tag{24}$$

$$\langle r|E^+\rangle = \frac{\sqrt{\varrho^+(k)}}{\mathcal{J}_+(k)}\, \chi(r;k)\,, \tag{25}$$

$$\langle r|E^-\rangle = \frac{\sqrt{\varrho^-(k)}}{\mathcal{J}_-(k)}\,\chi(r;k)\,. \tag{26}$$

As noted above, the analytical properties of the functions that multiply $\chi(r;E)$ in (24)–(26) is what ultimately leads to different RSPs. However, it is not always true that multiplying $\chi(r;E)$ by a function of $E$ yields an eigensolution that generates a different RSP. For instance, the radial solution $\chi(r;E)$ and the eigenfunction $\langle r|E\rangle$ both lead to the same RSP. This is why we say that $\langle r|E\rangle$ is the $\delta$-normalization of $\chi(r;E)$. In this case, $\sqrt{\varrho(k)}$ is just a normalization factor.

We may then ask: given the regular solution $\chi(r;E)$ and a function of the energy $f(E)$, how can we know whether $f(E)\chi(r;E)$ is just a normalization of $\chi(r;E)$ or leads to a different RSP? A general answer to this question is not known. Of course, to know the answer one can always apply the Sturm-Liouville theory and see if $f(E)\chi(r;E)$ yields the same RSP as $\chi(r;E)$. This may be impractical, though. A faster method, that works at least for simple potentials [1,15], is to check whether

$$[f(E^*)]^* = f(E)\,, \quad E \in \mathbb{C}\,, \tag{27}$$

or

$$[f(E^*)]^* \neq f(E)\,, \quad E \in \mathbb{C}\,. \tag{28}$$

If $f(E)$ fulfills (27), then $f(E)\chi(r;E)$ is just a normalization of $\chi(r;E)$. If $f(E)$ fulfills (28), then $f(E)\chi(r;E)$ and $\chi(r;E)$ lead to different RSPs and therefore have different physical content.

To check that the criterion (27)–(28) does indeed work for the spherical shell potential, we apply it to $\langle r|E\rangle$, $\langle r|E^+\rangle$, $\langle r|E^-\rangle$. We need first to choose the following branch for the square root function:

$$\sqrt{\cdot}: \{E \in \mathbb{C} \mid -\pi < \arg(E) \leq \pi\} \longmapsto \{E \in \mathbb{C} \mid -\pi/2 < \arg(E) \leq \pi/2\}\,. \tag{29}$$

For $\langle r|E\rangle$, one can easily check that

$$[\varrho(E^*)]^* = \varrho(E)\,, \quad E \in \mathbb{C}\,. \tag{30}$$

From (24) and (30), and from the criterion (27)–(28) it follows that $\langle r|E\rangle$ is just a normalization of $\chi(r;E)$. For $\langle r|E^+\rangle$, we have that

$$[\varrho^+(E^*)]^* = \varrho^+(E)\,, \quad E \in \mathbb{C}\,, \tag{31}$$

but

$$[\mathcal{J}_+(E^*)]^* = \mathcal{J}_-(E) \neq \mathcal{J}_+(E)\,, \quad E \in \mathbb{C}\,. \tag{32}$$

From (25), (31) and (32), and from the criterion (27)–(28) it follows that $\langle r|E^+\rangle$ is not a normalization of $\chi(r;E)$ but rather has a different physical content. Similarly, it can be seen that the physical content of $\langle r|E^-\rangle$ is not the same as that of $\langle r|E\rangle$.

### 2.3 Gamow Eigenfunctions

The Gamow vectors are the state vectors of resonances [5–10,1]. Like the standing-wave and the Lippmann-Schwinger eigensolutions, they solve the Schrödinger equation. At infinity, however, the Gamow eigenfunctions satisfy a boundary condition that is different from those satisfied by $\langle r|E\rangle$, $\langle r|E^{+}\rangle$, $\langle r|E^{-}\rangle$: the purely outgoing boundary condition. This purely outgoing behavior determines the physical content of the Gamow vectors.

There are two kinds of Gamow vectors. The first kind is the so-called decaying Gamow ket $|z_{\rm R}^{-}\rangle$, which is associated to a complex energy $z_{\rm R}=E_{\rm R}-{\rm i}\Gamma_{\rm R}/2$ that lies in the lower half plane of the second sheet of the Riemann surface. The corresponding wave number lies in the fourth quadrant of the complex wave-number plane. The second kind of Gamow vector is the so-called growing Gamow ket $|z_{\rm R}^{*}{}^{+}\rangle$, which is associated to an energy $z_{\rm R}^{*}=E_{\rm R}+{\rm i}\Gamma_{\rm R}/2$ that lies in the upper half plane of the second sheet of the Riemann surface. The corresponding wave number lies in the third quadrant of the complex wave-number plane. As far as the time-independent Schrödinger equation is concerned, any complex number can be an eigenvalue of the Hamiltonian [18]. The role of the purely outgoing boundary condition is to select, among all the complex energies, those that are to correspond to resonance energies [9].

In order to obtain the Gamow vectors, we solve the Schrödinger differential equation

$$\left(-\frac{\hbar^2}{2m}\frac{{\rm d}^2}{{\rm d}r^2}+V(r)\right)\langle r|z_{\rm R}\rangle = z_{\rm R}\langle r|z_{\rm R}\rangle\,, \tag{33}$$

subject to purely outgoing boundary conditions:

$$\langle 0|z_{\rm R}\rangle = 0 \tag{34a}$$

$$\langle r|z_{\rm R}\rangle \text{ is continuous at } r=a \text{ and at } r=b \tag{34b}$$

$$\frac{\rm d}{{\rm d}r}\langle r|z_{\rm R}\rangle \text{ is continuous at } r=a \text{ and at } r=b \tag{34c}$$

$$\langle r|z_{\rm R}\rangle \sim {\rm e}^{{\rm i}k_{\rm R}r} \text{ as } r\to\infty\,, \tag{34d}$$

where

$$k_{\rm R}=\sqrt{\frac{2m}{\hbar^2}z_{\rm R}}\;,\quad Q_{\rm R}=\sqrt{\frac{2m}{\hbar^2}(z_{\rm R}-V_0)}\;. \tag{35}$$

In (33) and (34a)–(34d), $\langle r|z_{\rm R}\rangle$ can denote either $\langle r|z_{\rm R}^{-}\rangle$ or $\langle r|z_{\rm R}^{*}{}^{+}\rangle$. This will cause no confusion, because whenever the complex energy lies in the lower half plane, $\langle r|z_{\rm R}\rangle$ will denote $\langle r|z_{\rm R}^{-}\rangle$, and whenever it lies in the upper half plane, $\langle r|z_{\rm R}\rangle$ will denote $\langle r|z_{\rm R}^{*}{}^{+}\rangle$.

For the spherical shell potential, (33) subject to the boundary conditions (34a)–(34d) has solutions only for a denumerable set of complex energies. These energies come in complex conjugate pairs $z_n$, $z_n^*$, where $z_n=E_n-{\rm i}\Gamma_n/2$ is the decaying pole, and $z_n^*=E_n+{\rm i}\Gamma_n/2$ is the growing pole. The corresponding decaying and growing wave numbers are given by

$$k_n=\sqrt{\frac{2m}{\hbar^2}z_n}\;,\quad -k_n^*=\sqrt{\frac{2m}{\hbar^2}z_n^*}\;,\quad n=1,2,\ldots \tag{36}$$

In terms of the wave number $k_n$, the $n$th decaying Gamow eigensolution reads

$$\langle r|z_n^-\rangle = N_n \begin{cases} \frac{1}{\mathcal{J}_3(k_n)} \sin(k_n r) & 0<r<a \\ \frac{\mathcal{J}_1(k_n)}{\mathcal{J}_3(k_n)} \mathrm{e}^{\mathrm{i}Q_n r} + \frac{\mathcal{J}_2(k_n)}{\mathcal{J}_3(k_n)} \mathrm{e}^{-\mathrm{i}Q_n r} & a<r<b \\ \mathrm{e}^{\mathrm{i}k_n r} & b<r<\infty\,, \end{cases} \tag{37}$$

where $N_n$ is a normalization factor,

$$N_n^2 = \mathrm{i}\,\mathrm{res}\left[S(k)\right]_{k=k_n} \,, \tag{38}$$

and where

$$Q_n = \sqrt{\frac{2m}{\hbar^2}(z_n - V_0)} \,. \tag{39}$$

The $n$th growing Gamow eigensolution reads

$$\langle r|z_n^{*+}\rangle = M_n \begin{cases} \frac{1}{\mathcal{J}_3(-k_n^*)} \sin(-k_n^* r) & 0<r<a \\ \frac{\mathcal{J}_1(-k_n^*)}{\mathcal{J}_3(-k_n^*)} \mathrm{e}^{\mathrm{i}Q_n^* r} + \frac{\mathcal{J}_2(-k_n^*)}{\mathcal{J}_3(-k_n^*)} \mathrm{e}^{-\mathrm{i}Q_n^* r} & a<r<b \\ \mathrm{e}^{-\mathrm{i}k_n^* r} & b<r<\infty\,. \end{cases} \tag{40}$$

where $M_n$ is a normalization factor,

$$M_n^2 = \mathrm{i}\,\mathrm{res}\left[S(k)\right]_{k=-k_n^*} = (N_n^2)^* \,, \tag{41}$$

and where

$$Q_n^* = \sqrt{\frac{2m}{\hbar^2}(z_n^* - V_0)} \,. \tag{42}$$

We compare now the boundary conditions (34a)–(34d) satisfied by the Gamow eigenfunctions with those satisfied by the standing-wave eigenfunctions [see (5a)–(5c)] and by the Lippmann-Schwinger eigenfunctions [see (17a)–(17e)]. Clearly, the boundary condition that is specific to the Gamow vectors is (34d). This boundary condition singles out the complex resonance spectrum of the Schrödinger equation by specifying the asymptotic behavior of the Gamow eigenfunctions. Moreover, the resonance spectrum selected by (34d) coincides with the poles of the $S$ matrix (18).

To finish this section, we note that in the $S$-matrix formalism, a resonance energy is reached by analytic continuation of $S(E)$ from its values on the physical spectrum to the resonance pole. In a similar vein, Gamow vectors can be viewed as the solutions of the analytic continuation of the Schrödinger equation [subject to the boundary conditions (34a)–(34d)] from the energies in the physical spectrum to the complex resonance eigenvalue.

## 3 The Arrow of Time of Quantum Electrodynamics

We have seen how boundary conditions determine the physical content of the eigensolutions of the time-independent Schrödinger equation. We now turn to see how boundary conditions affect the physical content of the solutions of the time-dependent Schrödinger equation. We shall see that time-asymmetric boundary conditions imposed upon the (time-symmetric) Schrödinger equation yield solutions that have an arrow of time built into them. Quantum Electrodynamics (QED) will be used as an illustrative example.

In order to make a parallel with the quantum case, we recall first the essential features of the arrow of time of Classical Electrodynamics (CED). The Maxwell equations, which describe the classical electromagnetic fields, are time symmetric. The solutions of the Maxwell equations can be written as a combination of a retarded and an advanced solution. Experimentally, we always observe that light has a retarded behavior – light cannot be detected at a distance $R$ from the source at any time less than $R/c$. In order to account for this retarded behavior, we select the retarded solution of the Maxwell equation and forbid the advanced solution. This amounts to imposing a time-asymmetric, retarded, causal boundary condition upon the (time-symmetric) Maxwell equations. Essentially, this is the radiation arrow of time. We stress that this arrow of time stems ultimately from the imposition of a causal boundary condition.

QED is the quantum counterpart of CED, and also has an arrow of time built into it. The arrow of time of QED is built into the Feynman propagator. Although the Schrödinger equation is time symmetric, one always imposes Feynman's $+\mathrm{i}\varepsilon$ prescription to construct the Feynman propagator – particles travel forward in time, whereas antiparticles "travel backward" in time [13]. Thus Feynman's $+\mathrm{i}\varepsilon$ prescription imposes a retarded (advanced) condition on the time evolution of particles (antiparticles). Essentially, this is the arrow of time of QED. In particular, this arrow of time sheds light onto the physical meaning of Feynman's $+\mathrm{i}\varepsilon$ prescription: this prescription is just a causal boundary condition imposed upon the time evolution of particles and antiparticles.

The example of QED can be generalized to any closed quantum system. Although the Schrödinger equation (which describes the evolution of a closed quantum system) is time symmetric, physical processes seem to comply with our basic notions of causality: cause is prior to effect. In order to make the solutions of the (time-symmetric) Schrödinger equation comply with causality, we impose causal, time-asymmetric boundary conditions upon the Schrödinger equation. These boundary conditions single out the causal solutions that account for the observed time-asymmetric phenomena. Building that (e.g., retarded) boundary condition into the time evolution of the quantum system involves the construction of an (e.g., retarded) propagator. Actually, although it is well known that propagators have an arrow of time built into them, it is not so well emphasized [11] that this implies the existence of a fundamental time asymmetry at the microscopic level.

Many authors have realized the central role played by boundary conditions in the description of time asymmetry. For example, Ritz [19] thought that the time asymmetry (often called irreversibility) of statistical mechanics arises from boundary conditions (in contrast to Einstein [19], who thought that irreversibility comes from averaging over a large number of systems, that is, for Einstein irreversibility emerges from probability and statistics). For Peierls [20] irreversibility also arises as a consequence of boundary conditions. To show this, Peierls rephrases Boltzmann's Stosszahl-Ansatz, which is the origin of the irreversibility of the so-called "Lorentz gas," as a boundary condition [20]. Some authors such as Penrose [21] or Gell-Mann and Hartle [22] have used boundary conditions as a possible explanation of time asymmetry, and even of time symmetry [22]. Other authors such as Preskill [23] also use boundary conditions to explain the time asymmetry (irreversibility) of quantum statistical mechanics: essentially, the non-decreasing behavior of the entropy can be understood as stemming from the assumption that system and environment are initially uncorrelated, i.e., from the assumption that the initial system-environment state is separable (unentangled) [23].

## 4 Conclusions

We have seen how important boundary conditions are in obtaining the solutions of the time-independent Schrödinger equation that fit a given physical situation. Essentially, the asymptotic behavior of the eigensolution determines its physical content. We have analyzed and compared the standing-wave, "in," "out," and purely outgoing boundary conditions. We have seen that the standing-wave, "in," and "out" boundary conditions yield three physically different RSPs. The purely outgoing boundary condition selects the resonance spectrum.

We have discussed the time-asymmetry of QED. Essentially, Feynman's $+i\varepsilon$ prescription, which is used to construct the Feynman propagator, encodes the time asymmetry of QED. We have also concluded that in general, the time evolution of a closed quantum system has a time asymmetry built into the propagators.

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## References

1. R. de la Madrid: Quantum Mechanics in Rigged Hilbert Space Language. PhD Thesis, Universidad de Valladolid, Valladolid (2001). Available at `http://www.isi.it/~rafa/`.
2. E. Brändas, M. Rittby, N. Elander: J. Math. Phys. **26**, 2648 (1985).

3. E. Engdahl, E. Brändas, M. Rittby, N. Elander: Phys. Rev. A **37**, 3777 (1988).
4. Obviously, the Hamiltonian has more RHS properties than those included in our definition of RSP.
5. G. Gamow: Z. Phys. **51**, 204 (1928).
6. A. F. J. Siegert: Phys. Rev. **56**, 750 (1939).
7. E. Hernández, A. Mondragón: Phys. Rev. C **29**, 722 (1984); A. Mondragón, E. Hernández, J. M. Velázquez Arcos: Ann. Phys. **48**, 503 (1991).
8. M. Baldo, L. S. Ferreira, L. Streit: Phys. Rev. C **36**, 1743 (1987); L. S. Ferreira, E. Maglione, R. J. Liotta: Phys. Rev. Lett. **78**, 1640 (1997).
9. R. de la Madrid, M. Gadella: Am. J. Phys. **70**, 626 (2002); quant-ph/0201091.
10. A. Bohm, M. Gadella: *Dirac kets, Gamow Vectors and Gelfand Triplets* (Springer Lecture Notes in Physics, **348**, Springer, Berlin 1989).
11. For a comprehensive overview of time symmetry and asymmetry, and of the arrow of time see: *Physical Origins of Time Asymmetry*, ed. by J. J. Halliwell, J. Pérez-Mercader, W. H. Zurek (Cambridge University Press, Cambridge 1994).
12. L. I. Schiff: *Quantum Mechanics* (McGraw-Hill, New York 1968).
13. R. P. Feynman: *Quantum Electrodynamics* (Benjamin, New York 1961).
14. N. Dunford, J. Schwartz: *Linear operators*, vol. II (Interscience Publishers, New York 1963).
15. R. de la Madrid: J. Phys. A: Math. Gen. **35**, 319 (2002); quant-ph/0110165.
16. R. de la Madrid: Chaos, Solitons & Fractals **12**, 2689 (2001); quant-ph/0107096.
17. R. de la Madrid, A. Bohm, M. Gadella: Fortsch. Phys. **50**, 185 (2002); quant-ph/0109154.
18. This is in no contradiction with the self-adjointness of the Hamiltonian, because the eigensolutions that correspond to complex eigenvalues lie outside the Hilbert space.
19. R. Ritz: Physikalische Zeitschrift **9**, 903 (1908); *ibid.* **10**, 224 (1909); R. Ritz, A. Einstein: Physikalische Zeitschrift **10**, 323 (1909).
20. R. Peierls: *Surprises in Theoretical Physics* (Princeton University Press, Princeton 1979).
21. R. Penrose: 'Singularities and time-asymmetry'. In *General Relativity: An Einstein Centenary Survey*, ed. by S. W. Hawking, W. Israel (Cambridge University Press, Cambridge 1979), pp. 581-638.
22. M. Gell-Mann, J. B. Hartle: 'Time Symmetry and Asymmetry in Quantum Mechanics and Quantum Cosmology'. In [11], pp. 311-345.
23. J. Preskill: *Physics 229: Advanced Mathematical Methods of Physics – Quantum Computation and Information* (California Institute of Technology, Pasadena, CA, 1998). Available at `http://www.theory.caltech.edu/people/preskill/ph229/`.